

2-(Methylsulfanyl)quinoxaline
21948-73-2 | DTXSID00325902

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 282 °C

Global applicability domain: Inside

Local applicability domain index: 4.37e-01

Confidence level: 6.11e-01

Nearest Neighbors from the Training Set

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1H-Pyrazole, 3,5-dimethyl-1-phenyl-

Measured: 273

Predicted: 287

Image not found

3-Methyl-1-phenyl-1H-pyrazole

Measured: 255

Predicted: 275

Image not found

1H-Benzimidazole, 1-ethyl-2-methyl-

Measured: 296

Predicted: 270

Image not found

1-Phenylimidazole

Measured: 276

Predicted: 273

Image not found

Phthalazine

Measured: 316

Predicted: 263